

Interplay of disorder and spin fluctuations in the resistivity near a quantum critical point

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The resistivity in metals near an antiferromagnetic quantum critical point (QCP) is strongly affected by small amounts of disorder. In a quasi-classical treatment, we show that an interplay of strongly anisotropic scattering due to spin fluctuations and isotropic impurity scattering leads to a large regime where the resistivity varies as T^α , with an anomalous exponent, α , $1 \lesssim \alpha \lesssim 1.5$, depending on the amount of disorder. I argue that this mechanism explains in some detail the anomalous temperature dependence of the resistivity observed in CePd₂Si₂, CeNi₂Ge₂ and CeIn₃ near the QCP.

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In the last five years an increasing number of heavy-fermion metals near an antiferromagnetic (AFM) quantum critical point was shown to display striking deviations from conventional Fermi-liquid behavior [1–4]. A few of the dirtier systems (e.g. [4]) appeared to show the $T^{3/2}$ behavior of the resistivity, $\rho(T)$, as predicted by the Hertz-Millis spin-fluctuation theory for such a QCP [5–7]. In other cleaner single-crystal systems, such as CePd₂Si₂, CeNi₂Ge₂ and CeIn₃ [2,3], $\rho(T)$ varies as T^α with exponents α between 1.1 and 1.5. It has been argued [8] that such a behavior signals a fundamental breakdown of Fermi liquid theory.

In this letter we propose a simple theoretical explanation for this anomalous behavior which covers both dirty and clean systems. Our main result is that the resistivity anomalies mentioned above can be attributed to the interplay between quantum-critical AFM spin fluctuations [5,6] and impurity scattering in a conventional Fermi liquid. In fact, the resistivity can be described in semi-quantitative terms in the context of the simplest semi-classical Boltzmann equation approach. Here, we will have nothing to say about the striking linear behavior of $\rho(T)$ near the QCP in CeCu_{6-x}Au_x [1] in which the neutron scattering experiments suggest a more unconventional behavior of the spin-fluctuations [9].

The temperature dependence of $\rho(T)$ can already be understood from the following qualitative argument: First we recall that scattering off AFM spin-fluctuations is most effective near “hot lines”, i.e., points at the Fermi surface connected by the ordering wave vector \mathbf{Q} (see Fig. 1) where gaps would open up in the antiferromagnetically ordered (metallic) phase. As explained by Hlubina and Rice [10], the strong scattering near these lines is short circuited by the “cold” regions on the Fermi surface, where the scattering rates are small. In clean systems the latter dominate the transport and resistivity acquires the usual Fermi liquid behavior, $\rho(T) \sim T^2$ at sufficiently low temperatures. Impurity scattering leads essentially to an averaging of the scattering rate over the Fermi surface re-

ducing the effectiveness of the Hlubina-Rice mechanism and emphasizing the role of the “hot lines”. The above line of argumentation can be made more quantitative: Near the “hot lines” the scattering rate $1/\tau_S$ of the quasi-particles due to the quantum-critical spin-fluctuations is linear in temperature $\tau_M/\tau_S \approx t = T/\Gamma$ where Γ is a characteristic energy scale and τ_M a typical scattering time. The width of these “hot lines” is given by \sqrt{t} (see below). In the “cold regions”, we expect Fermi liquid behavior with $\tau_M/\tau_S \approx t^2$. Weak disorder leads to an isotropic scattering rate, $1/\tau_{el} = x/\tau_M$, where x is a small dimensionless number measuring the effectiveness of impurity compared to magnetic scattering ($x^{-1} \approx k_F l$ for spin-fluctuation scattering in the strong coupling “unitarity” limit; l is the elastic mean-free-path). The conductivity σ is proportional to the average of $\tau_{\mathbf{k}}$ over the Fermi surface (FS) with $1/\tau_{\mathbf{k}} = 1/\tau_{el} + 1/\tau_S(\mathbf{k})$:

$$\sigma \propto \langle \tau_{\mathbf{k}} \rangle_{\text{FS}} \propto \frac{\sqrt{t}}{x+t} + \frac{1-\sqrt{t}}{x+t^2}. \quad (1)$$

The two terms describe the contributions from “hot” and “cold” regions, respectively. For $x < t^2 < 1$ cold regions short-circuit the hot ones and from the second term in (1) we obtain $\rho \propto t^2$ [10]; while for $t < x < 1$, the hot spots dominate and the resistivity $1/\sigma$ is proportional to $x + t^{3/2}$. At intermediate temperatures, $x < t < \sqrt{x}$, we expect a crossover regime, in which we can define an effective resistivity exponent α , in terms of the logarithmic difference of $\Delta\rho(T) = \rho(T) - \rho(0)$ at the crossover temperatures $T_1^c = \Gamma x$ and $T_2^c = \Gamma\sqrt{x}$,

$$\alpha \approx \frac{\ln \Delta\rho(T_2^c) - \ln \Delta\rho(T_1^c)}{\ln T_2^c - \ln T_1^c} \approx \frac{\ln x - \ln x^{3/2}}{\ln \sqrt{x} - \ln x} = 1. \quad (2)$$

In a very clean system this crude estimate implies a nearly linear crossover behavior in temperature as measured in clean samples of CePd₂Si₂ and CeNi₂Ge₂ [2,3].

We now proceed with a more precise argument based on the semi-classical Boltzmann equation treatment of

electrons interacting with spin-fluctuations and impurities. The former are described by a theory above the upper critical dimension [5,6] and, due to the ohmic damping of the magnetic excitations in a metal, is characterized by a dynamical exponent $z = 2$. As a result, the spin-fluctuation spectrum can be modeled by [5,6]

$$\chi_{\mathbf{q}}(\omega) = \chi_{-\mathbf{q}}(\omega) \approx \frac{1}{1/(q_0\xi)^2 + (\mathbf{q} \pm \mathbf{Q})^2/q_0^2 - i\omega/\Gamma}, \quad (3)$$

where q_0 and Γ are characteristic momentum and energy scales; and ξ is the AFM correlation length which, at the QCP, diverges as $1/\xi^2 \approx cq_0^2(T/\Gamma)^{3/2}$ [5,6]. For the purposes of our numerical calculations we set $c = 1$ (c does not influence the low-temperature properties).

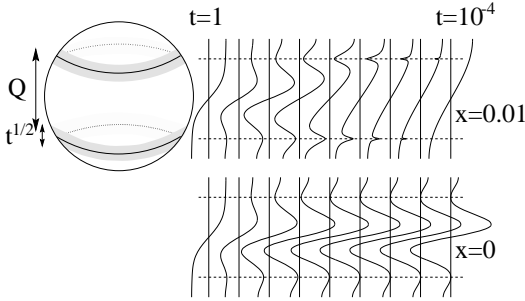


FIG. 1. Near the transition to an antiferromagnet with ordering vector \mathbf{Q} , the scattering on the Fermi-surface is enhanced along “hot lines” connected by \mathbf{Q} . The width of this region is given by $\Delta k \approx q_0\sqrt{T/\Gamma}$. The out-of-equilibrium distribution Φ_θ of the quasi particles for a current parallel to \mathbf{Q} is shown as a function of the azimuthal angle θ for temperatures ranging from $t = (q_0/k_F)^2(T/\Gamma)^2 = 1$ (left) down to $t = 10^{-4}$ (right) and for both a clean system (lower curves) and a small amount of disorder, $x = 0.01$ (upper curves).

Our starting point is the Boltzmann equation with a quasi-particle distribution function $f_{\mathbf{k}} = f_{\mathbf{k}}^0 - \Phi_{\mathbf{k}}(\partial f_{\mathbf{k}}^0/\partial \epsilon_{\mathbf{k}})$ linearized around the Fermi distribution $f_{\mathbf{k}}^0$ with a collision term

$$\left. \frac{\partial f_{\mathbf{k}}}{\partial t} \right|_{\text{coll}} = \sum_{\mathbf{k}'} \frac{f_{\mathbf{k}'}^0(1-f_{\mathbf{k}}^0)}{T} (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'}) \times \left[g_{\text{imp}}^2 \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'} + \frac{2g_S^2}{\Gamma} n_{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}^0 \text{Im}\chi_{\mathbf{k}-\mathbf{k}'}(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) \right] \quad (4)$$

Here g_{imp}^2 and g_S^2 are transition rates for isotropic impurity scattering and inelastic scattering from spin fluctuations, respectively, and n_ω^0 is the Bose function. Eqn. (4) tacitly assumes that the spin-fluctuations stay in equilibrium, an approximation valid if the spin fluctuations can lose their momentum effectively by Umklapp or impurity scattering. Instead of solving the Boltzmann equation directly, it is instructive to consider a mathematically equivalent variational principle [12]. Following Hlubina and Rice [10], we define a functional ρ of $\Phi_{\mathbf{k}}$

$$\rho[\Phi_{\mathbf{k}}] = \frac{\hbar}{4e^2} \frac{\oint \oint \frac{d\mathbf{k}d\mathbf{k}'}{v_{\mathbf{k}}v_{\mathbf{k}'}} F_{\mathbf{k}\mathbf{k}'} (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'})^2}{\left(\oint \frac{d\mathbf{k}}{v_{\mathbf{k}}} (\mathbf{v}_{\mathbf{k}} \mathbf{n}) \Phi_{\mathbf{k}} \right)^2} \rightarrow \min \quad (5)$$

$$F_{\mathbf{k}\mathbf{k}'} = g_{\text{imp}}^2 + \frac{2g_S^2}{\Gamma T} \int_0^\infty \omega n_\omega^0 [n_\omega^0 + 1] \text{Im}\chi_{\mathbf{k}-\mathbf{k}'}(\omega) d\omega. \quad (6)$$

The physical resistivity is given by the minimum of $\rho[\Phi_{\mathbf{k}}]$ regarded as a functional of $\Phi_{\mathbf{k}}$. At this minimum $\Phi_{\mathbf{k}}$ is directly proportional to the true distribution function in an electric field applied in the direction of the unit vector \mathbf{n} . In the above expression only integrals over the Fermi surface enter, as we have already integrated out the perpendicular components of \mathbf{k} by using $\int d\epsilon_{\mathbf{k}} \oint d\mathbf{k}/v_{\mathbf{k}}$ where $v_{\mathbf{k}}$ is the velocity of quasi particles at the Fermi surface.

In the following we simplify the discussion by (i) considering a spherical Fermi surface and (ii) limiting ourselves to transport parallel to the ordering wave vector $\mathbf{Q} = (0, 0, 2k_F \cos \theta_H)$, in which case $\Phi_{\mathbf{k}} = \Phi_\theta$ is only a function of the azimuthal angle θ . The equations $\theta = \theta_H$ and $\theta = \pi - \theta_H$ define the “hot lines” shown in Fig. 1. The geometry [11] and precise value of θ_H are not very important as long as one stays away from $\theta_H = 0$ (“ $2k_F$ ” ordering) or $\theta_H = \pi/2$ (ferromagnetic ordering) where our approach breaks down [6]; in our numerical calculations we use $\theta_H = \pi/6$. As in [10] we approximate the second term in Eqn. (6) by $2g_S^2 I[y]$ with $I[y] \approx \pi^2/(y(3y+2\pi))$ and $y = (\Gamma/T) (1/(q_0\xi)^2 + (\mathbf{q} \pm \mathbf{Q})^2/q_0^2)$ which is asymptotically exact for large and small y .

After performing the integration over ω and the polar angle φ in Eqn. (5) we obtain

$$\rho(T) = \min[\rho_{\text{imp}}[\Phi_\theta] + \rho_S[\Phi_\theta]] \quad (7)$$

$$\rho_{\text{imp}} = \frac{x\rho_M}{6} \frac{\iint_0^\pi (\Phi_{\theta_1} - \Phi_{\theta_2})^2 \sin \theta_1 d\theta_1 \sin \theta_2 d\theta_2}{\left(\int_0^\pi \cos \theta \Phi_\theta \sin \theta d\theta \right)^2} \quad (8)$$

$$\rho_S = \frac{\pi\rho_M}{3} \frac{\iint_0^\pi F_{\theta_1\theta_2} (\Phi_{\theta_1} - \Phi_{\theta_2})^2 \sin \theta_1 d\theta_1 \sin \theta_2 d\theta_2}{\left(\int_0^\pi \cos \theta \Phi_\theta \sin \theta d\theta \right)^2} \quad (9)$$

where $\rho_M = 3\hbar g_S^2/(e^2 v_F^2)$ is a typical resistivity due to scattering from spin fluctuations at approximately the temperature scale Γ and $x = g_{\text{imp}}^2/(2g_S^2)$ measures the relative strength of impurity scattering. The prefactors are chosen in such a way that $x\rho_M = 3\hbar g_{\text{imp}}^2/(2e^2 v_F^2)$ is the residual resistivity. The dimensionless scattering rate $F_{\theta_1\theta_2}$ averaged over the polar angle φ is given by

$$F_{\theta_1\theta_2} \approx \int_0^{2\pi} \frac{d\varphi}{2\pi} I[y(\theta_1, \theta_2, \varphi)] \quad (10)$$

$$\approx \frac{\pi t^2/(2 \sin \theta_H)}{|\Delta\vartheta| \left(2t + \frac{3}{\pi} \left((\Delta\vartheta)^2 + |\Delta\vartheta| \sqrt{(\Delta\vartheta)^2 + \frac{2\pi t}{3}} \right) \right)}$$

$$(\Delta\vartheta)^2 = \vartheta_1^2 + \vartheta_2^2 + 2\vartheta_1\vartheta_2 \cos 2\theta_H + 1/(k_F\xi)^2$$

$\vartheta_1 = \theta_1 - \theta_H$ and $\vartheta_2 = \theta_2 - (\pi - \theta_H)$ measure the distances from the “hot lines” and $t = (T/\Gamma)(q_0/k_F)^2$ is the

dimensionless temperature. Our numerical calculations use the full polar integral in (10), even though at low temperatures, $(1/(\xi k_F)^2, t \ll 1)$ the correct behavior is also contained in the approximate form.

From Eqns. (7)–(10) one can easily deduce the qualitative behavior of the low-temperature resistivity. We first consider the case of very low temperatures in a dirty metal. In this regime the resistivity is dominated by the disorder contribution ρ_{imp} . From $\delta\rho_{\text{imp}}[\Phi_\theta]/\delta\Phi_\theta = 0$ we find the usual quasi-particle distribution for impurity scattering $\Phi_\theta = \cos\theta$. The leading temperature independent correction to the residual resistivity $\rho_0 = x\rho_M$ is then given by $\rho_S[\cos\theta]$. The main contribution to ρ_S arises in a small region around the hot spots, where $(\Phi_{\theta_1} - \Phi_{\theta_2})^2 \approx (\cos\theta_H - \cos(\pi - \theta_H))^2$ is finite. Scaling $\vartheta_{1/2}$ in Eqn. (10) with \sqrt{t} one recognizes that in the regime $t > 1/(k_F\xi)^2 \propto t^{3/2}$ the finite correlation length can be neglected and at lowest temperatures the resistivity is given by

$$\rho(T \rightarrow 0) = \rho_M \left[x + \sqrt{\frac{3\pi^7}{8}} \frac{q_0^3 \cos\theta_H}{k_F^3} \left(\frac{T}{\Gamma} \right)^{3/2} \right]. \quad (11)$$

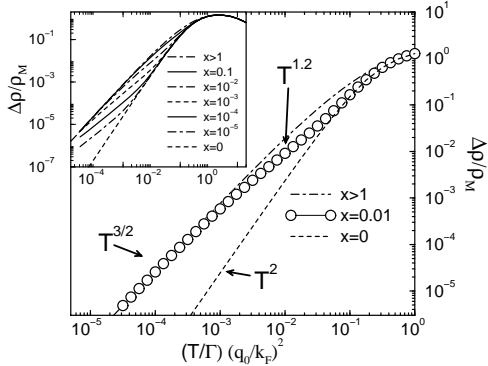


FIG. 2. Log-log plot of $\Delta\rho = \rho(T) - \rho(0)$ for a rather clean system with $x = 0.01$. Note the large crossover regime from the resistivity of a clean system (dashed line) at high temperatures to the resistivity of a dirty system (dot-dashed line). The inset shows, how this crossover evolves for various impurity concentrations x .

On the other hand, if the system is clean ($x = 0$), we have to minimize $\rho_S[\Phi_\theta]$. As pointed out by Hlubina and Rice [10], the ansatz $\Phi_\theta = \cos\theta$ is far from the true minimum. We can considerably reduce ρ_S by using a distribution function where the “hot lines” are excluded, e.g. $\Phi_\theta = 0$ for $|\theta - \theta_H| < \theta_{\text{cut}}$ and $|\theta - (\pi - \theta_H)| < \theta_{\text{cut}}$. For this ansatz, the temperature dependence in the numerator of the scattering rate (10) can be neglected for $\theta_{\text{cut}} \gg \sqrt{t}$ and the resistivity is given by

$$\rho(x = 0, T \rightarrow 0) = c\rho_M(q_0/k_F)^2(T/\Gamma)^2 \quad (12)$$

where c is a non-universal number of order 1 which depends on the details of the scattering mechanism in the “cold regions” of the Fermi surface.

To obtain the crossover behavior we calculate the distribution function Φ_θ and the resistivity $\rho(T)$ within our model numerically by solving the integral equation $\delta\rho[\Phi_\theta]/\delta\Phi_\theta = 0$ which is equivalent to solving the linearized Boltzmann equation directly. For a clean system, Φ_θ is shown in the lower part of Fig. 1. At high temperatures the distribution function is structureless and all parts of the Fermi surface (besides those perpendicular to the current) contribute more or less equally to the resistivity. However, for lower temperatures the region around the “hot lines” (dashed lines in Fig. 1) are short circuited and the distribution function vanishes. Accordingly the resistivity is much lower and drops $\propto T^2$ (dashed line in Fig. 2).

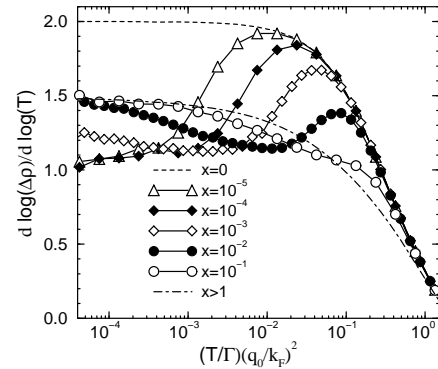


FIG. 3. Effective exponent of the resistivity, defined as the logarithmic derivative of $\Delta\rho(T)$. At very low temperatures, the “dirty-limit” exponent $3/2$ is recovered. However, in the experimentally accessible low temperature regime smaller exponents are to be expected for rather clean system ($x < 0.1$).

As shown in the simple calculation discussed in the beginning, in a system with a small amount of disorder, we expect a large crossover regime between the behavior described by Eqns. (11) and (12). In the variational approach given here this is due to the effect, that the impurity resistivity is *not* minimized by the distribution function $\Phi_\theta^{\text{clean}}$ (the low temperature curve in the lower part of Fig. 1) and $\rho_{\text{imp}}[\Phi_\theta^{\text{clean}}] = (1 + c')x\rho_M$, where c' is a number of order 1 (e.g. $c' \approx 2.8$ in our model). Below a temperature T_2^c , defined by $c'\rho(T = 0) \approx \rho(x = 0, T_2^c)$, the distribution function deviates from $\Phi_\theta^{\text{clean}}$ and approaches the $\cos\theta$ -form which minimizes impurity scattering (see Fig. 1). Qualitatively, we obtain the same picture as in the crude estimate discussed at the beginning (up to factors like c').

The evolution of this crossover regime with impurity concentration is shown in Fig. 2 and its inset. The dependence of the distribution function (and of $\Delta\rho$) on impurity-concentration is a reflection of the complete breakdown of Matthiessen’s rule in the crossover regime, where it is not possible to separate the different scattering mechanisms contributing to the resistivity. In addition, while not entirely physically meaningful, the $(T-$

dependent) effective exponent defined by the logarithmic derivative of $\rho(T) - \rho(0)$ in Fig. 3, when properly interpreted, displays the various crossovers in a dramatic way. For example, even for reasonably clean system either asymptotic exponents, 2 and 1.5 are difficult to observe, while effective exponents close to 1 dominate over a wide range of parameter values as suggested by our estimate (2).

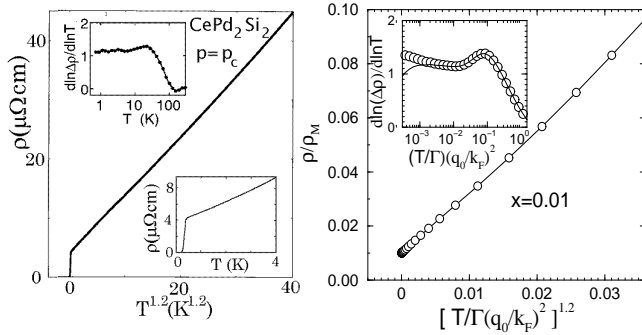


FIG. 4. Resistivity as a function of $T^{1.2}$ in CePd_2Si_2 taken from [2] (left figure) compared to our calculation (right figure) for $x = 0.01$. The insets show the corresponding logarithmic derivative of $\rho(T) - \rho(0)$. The solid line in the inset of the theoretical plot displays the logarithmic derivative of $\rho(T) - 0.995\rho(0)$. Below $\approx 400\text{mK}$ CePd_2Si_2 is superconducting (lower inset). Note the offset of the line $T = 0$ in both plots.

While the behavior for $1/(k_F\xi)^2, t \gtrsim 1$ are highly non-universal and strongly affected by details of the band structure and scattering mechanisms, this is not the case in the opposite limit $1/(k_F\xi)^2, t \ll 1$, which is of interest here. In the latter regime crossover effects depend only very weakly on the precise details of the model.

We argue that our approach explains the anomalous resistivity at the QCP observed in the very good samples of CePd_2Si_2 , CeNi_2Ge_2 and CeIn_3 [2,3]. In Fig. 4 we show the measurement by Grosche *et al.* [2] of the resistivity as a function of $T^{1.2}$ at the critical pressure in CePd_2Si_2 and compare them to our model for $x = 0.01$. It is important to note, that not only the same exponent of the resistivity shows up in the theory, but that it is also observed over a similar range $0.1\rho_0 \lesssim \Delta\rho(T) \lesssim 10\rho_0$. This suggests that standard spin-fluctuation theory [5–7] can be applied for this system opening the possibility for a theory of the striking superconducting phase observed below 400mK. In CeNi_2Ge_2 , a similar exponent is observed in the resistivity [2], while the effective exponents in samples of CeIn_3 [3] show a behavior reminiscent of our predictions for $x = 0.1$ in Fig. 3. It is certainly necessary to check other predictions of this theory carefully. For example, according to [6], the pressure dependence of the Néel temperature near the QCP should be given by $(p - p_c)^{2/3}$ while experimentally a linear dependence seems to be observed over some range [2]. Also the specific heat should give valuable informations on the nature

of the spin fluctuations. The most direct test of the effects described in this letter is, however, a comparison of the critical resistivity in samples of different quality. According to our theory, the effective exponent has to change from 1.5 for dirty samples to values near 1 for very clean samples. Also, for cleaner and cleaner samples, a “bump” has to show up in plots of the effective exponent (cf. Fig. 3). The dependence of the exponent on sample quality has indeed been reported [2].

For systems not directly at but still near the QCP ($k_F\xi(T = 0) \gg 1$), we expect again a large crossover regime in the resistivity with anomalous effective exponents due to a pronounced crossover from $\rho \approx \rho_M(T/T)^2$ at high temperatures to $\rho \approx \rho_M(x + (T/T)^2(k_F\xi))$ at lowest temperatures.

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